

Statistics dependence of the entanglement entropy

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The entanglement entropy of a distinguished region of a quantum many-body system reflects the entanglement present in its pure ground state. In this work, we establish scaling laws for this entanglement for *critical* quasi-free fermionic and bosonic lattice systems, without resorting to numerical means. We consider the geometrical setting of D -dimensional half-spaces which allows us to exploit a connection to the one-dimensional case. Intriguingly, we find a difference in the scaling properties depending on whether the system is bosonic—where an area-law is first proven to hold—or fermionic, extending previous findings for cubic regions. For bosonic systems with nearest neighbor interaction we prove the conjectured area-law by computing the logarithmic negativity analytically. We identify a length scale associated with entanglement, different from the correlation length. For fermions we determine the logarithmic correction to the area-law, which depends on the topology of the Fermi surface. We find that Lifshitz quantum phase transitions are accompanied with a non-analyticity in the prefactor of the leading order term.

The occurrence of critical points at zero temperature holds the key to the understanding of several phenomena in quantum many-body systems in the condensed matter context [1]. Quantum criticality is accompanied by a divergence of the typical length scale, the correlation length. These long-range correlations come along with genuine entanglement in the ground state, grasped by the entanglement entropy $E_S = S(\text{tr}_{\mathcal{A}}[\rho])$. This is the entropy of the reduced density matrix that is obtained when tracing out the degrees of freedom outside a distinguished region \mathcal{A} , quantifying the degree of entanglement between this region and the rest [2–19].

This notion of the entanglement or geometric entropy—and more to the point its scaling behavior abstracting from details of the model—has enjoyed a strong revival of interest recently, partially driven by intuition from quantum information theory: previously conjectured scaling laws in higher dimensions [2], relating the entanglement entropy to the boundary area—not the volume—of the region, have been rigorously established using quantum information ideas [4–6]. This was followed by observations of violations of such area-laws [7]. The entanglement entropy has in its non-leading-order behavior interestingly been linked to the topology of the system [8], using ideas of topological quantum field theory, and been studied under time evolution [9]. Partly, this renewed interest is triggered by the implications on the simulatability of quantum systems using density-matrix renormalization approaches: the entanglement entropy quantifies in a sense the relevant number of degrees of freedom to be considered [3, 10].

If entanglement is to reflect critical or non-critical properties of quantum many-body systems, an area-relationship might of course be expected to hold or not, depending on whether the two-point correlation functions diverge. One might be tempted to think that entanglement could yet be seen as an indicator of criticality in the same sense. Intriguingly, it turns out that the situation is more complex. As we will also see, even for critical systems, an area-relationship can hold, despite a divergent correlation length (as can also be observed in projected entangled pair states, satisfying an area-law by construction [11]). In this work, we demonstrate with a fully analytical argument that it can depend on the statistics of the

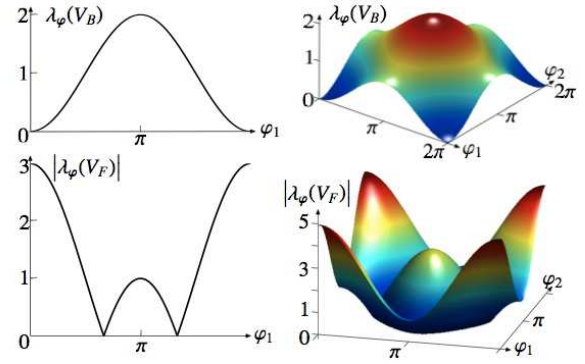


FIG. 1: Spectra of critical nearest-neighbour Hamiltonians (top: bosonic, bottom: fermionic) in one and two dimensions. The spectrum of the individual decoupled chains is given by the spectrum of the full Hamiltonian along the first coordinate φ_1 . The topology of the set of solutions to $\lambda_\varphi = 0$ —the Fermi-surface in the fermionic case—provides an intuition as to why the scaling behavior of entanglement is different for fermions then for bosons in $D > 1$, see text.

system—bosonic or fermionic—whether an area-relationship holds or is in fact violated. In this way, we resolve the key open question: “What happens in the critical bosonic case?” In the process we confirm some conjectures based on numerical findings for small system size [2, 12, 13] and refute others, such as the conjecture of a break-down of an area law for critical bosons in $D > 1$ in Ref. [14].

Here, we establish first analytical scaling laws for critical bosonic systems. We achieve these results for the geometrical setting of a half-space in D -dimensions, completing the program initiated in Ref. [5]. These findings are compared with fermionic half-spaces, complementing recent results on cubic regions in Refs. [7], and in a fashion consistent with numerical work in Ref. [12, 13]. We treat bosonic and fermionic systems on the same footing – in terms of Majorana operators for fermions and canonical coordinates for bosons. We hence provide a unified and complete framework for entanglement

scaling in critical quasi-free systems with that geometry.

The setting. – We consider cubic lattices of spatial dimension D , $\mathcal{L} = [1, \dots, N]^{\times D}$, $|\mathcal{L}| = N^D$, equipped with *periodic boundary conditions* and study ground states ϱ of Hamiltonians that are quadratic forms of either bosonic or fermionic operators. The geometric setting is that of a half-space, distinguishing w.l.o.g. the first spatial direction, considering a subsystem $\mathcal{A} = [1, \dots, M] \times \mathcal{L}'$, $\mathcal{L}' = [1, \dots, N]^{\times D-1}$, and its entanglement with the rest $\mathcal{B} = \mathcal{L} \setminus \mathcal{A} = [M+1, \dots, N] \times \mathcal{L}'$. We can hence make use of an idea of exploiting transverse momenta. This geometrical setting has notably numerically been assessed with respect to local spectra and simulatability issues in the seminal work Ref. [3].

When we say that (i) this entanglement as quantified by the von-Neumann entropy $E_S(M, N) = S(\varrho_{\mathcal{A}})$ of the reduced state $\varrho_{\mathcal{A}} = \text{tr}_{\mathcal{B}}[\varrho]$ satisfies an *area-law*, we mean that for $M = N/2$ the entanglement entropy satisfies

$$\mathcal{E} := \lim_{N \rightarrow \infty} E_S(M, N)/N^{D-1} \leq \text{const},$$

i.e., it scales at most like the *boundary area* of \mathcal{A} .

For systems *violating* the area-law, $\mathcal{E} = \infty$, we will (ii) study the exact form of the encountered logarithmic divergence in M ,

$$\mathcal{E} = \text{const} \times \log M + o(\log M).$$

We will subsequently discuss physical systems that are described by Hamiltonians of the type

$$\hat{H} = \frac{1}{2} \sum_{i,j} \left[\hat{d}_i^\dagger A_{i,j} \hat{d}_j + \hat{d}_i B_{i,j} \hat{d}_j^\dagger + \hat{d}_i C_{i,j} \hat{d}_j + \hat{d}_i^\dagger D_{i,j} \hat{d}_j^\dagger \right],$$

where operators \hat{d}_i are either bosonic or fermionic and vectors $\mathbf{i} = (i_1 \dots i_D) \in \mathcal{L}$ label individual sites of the cubic lattice. To ensure hermiticity we demand the real coefficients to satisfy $A_{i,j} = B_{i,j} = A_{j,i}$ and $C_{i,j} = D_{i,j} = C_{j,i}$ for bosons, and $A_{i,j} = -B_{i,j} = A_{j,i}$, $C_{i,j} = -D_{i,j} = -C_{j,i}$ for fermions. Furthermore, we assume translational invariance and periodic boundary conditions (all coupling matrices depend only on the difference $\mathbf{i} - \mathbf{j}$ and are cyclic matrices). We will lead the discussion in terms of hermitian operators $\hat{\mathbf{r}} = (\hat{x}_1, \dots, \hat{x}_{|\mathcal{L}|}, \hat{p}_1, \dots, \hat{p}_{|\mathcal{L}|})^t$ (in a mild abuse of notation, the transposition refers to the tuple, not to operators) defined by $\hat{x}_i = (\hat{d}_i + \hat{d}_i^\dagger)/\sqrt{2}$ and $\hat{p}_i = -i(\hat{d}_i - \hat{d}_i^\dagger)/\sqrt{2}$. In the bosonic case they are indeed position and momentum operators fulfilling the canonical commutation relations (CCR). In turn, for fermionic operators, they are so called *Majorana operators* fulfilling the canonical anti-commutation relations (CAR). We will assume isotropic couplings for fermions, $C = 0$, and coupling only in position for bosons, $A - C = \mathbb{1}$. In order not to obscure our main point, we will not consider the straightforward but cumbersome generalization to anisotropic or momentum couplings. The Hamiltonian now reads ($V_B := A + C$, $V_F := A$)

$$\hat{H}_B = \frac{1}{2} \hat{\mathbf{r}}^t \begin{bmatrix} V_B & 0 \\ 0 & \mathbb{1} \end{bmatrix} \hat{\mathbf{r}}, \quad \hat{H}_F = \frac{i}{2} \hat{\mathbf{r}}^t \begin{bmatrix} 0 & V_F \\ -V_F^t & 0 \end{bmatrix} \hat{\mathbf{r}} \quad (1)$$

for bosons and fermions, respectively. Whenever we may treat both species equally, we denote by V the coupling in position $V = V_B$ for bosons and $V = V_F$ for fermions.

Starting from the Hamiltonians above, their spectrum and respective ground states are found in the usual way by diagonalizing \hat{H}_B through symplectic transformations, transformations respecting the CCR, and \hat{H}_F by orthogonal transformations, transformations respecting the CAR. As matrices V are cyclic, the bosonic spectrum is given by $\lambda_{\mathbf{k}}$ and the fermionic spectrum by $|\lambda_{\mathbf{k}}|$, where $\lambda_{\mathbf{k}} = \sum_{l \in \mathcal{L}} V_l \cos(2\pi \mathbf{k} l / n)$, $\mathbf{k} \in \mathcal{L}$.

The half-space geometry allows for a transformation of both Hamiltonians to a system of mutually uncoupled one-dimensional chains while respecting the CCR and CAR, but notably, changing the local properties of the systems forming the individual chains. To this end consider the transformation $\hat{\mathbf{r}} = (\mathcal{O} \oplus \mathcal{O}) \hat{\mathbf{q}}$ to a new set of operators $\hat{\mathbf{q}}$, where the $|\mathcal{L}| \times |\mathcal{L}|$ matrix \mathcal{O} is given by $\mathcal{O}_{i,j} = \delta_{i_1, j_1} \mathcal{O}_{i', j'}$. Here and in the following we write vectors $\mathbf{i} = (i_1 \dots i_D) \in \mathcal{L}$ as $\mathbf{i} = (i_1 \mathbf{i}')$, $\mathbf{i}' = (i_2 \dots i_D) \in \mathcal{L}'$. Now, the transformation \mathcal{O} acts on the first coordinate as the identity and is thus local with respect to the bipartition $\mathcal{A}|\mathcal{B}$, i.e., it does not change entanglement properties. In order to respect the CAR and CCR the matrix \mathcal{O} needs to be orthogonal. Then, the Hamiltonians $\hat{H}_{B/F}$ read in coordinates $\hat{\mathbf{q}}$ just as in Eq. (1) with modified coupling matrices $V \mapsto \mathcal{O}^t V \mathcal{O}$. As cyclic matrices commute and may be diagonalized by the same Fourier transformation, we have the explicit form

$$V_l = \sum_{\mathbf{k}' \in \mathcal{L}'} \frac{\lambda_{\mathbf{k}'}(l_1) e^{2\pi i \mathbf{k}' \cdot l' / |\mathcal{L}'|}}{|\mathcal{L}'|}, \quad \lambda_{\mathbf{k}'}(l_1) = \sum_{k_1=1}^N \frac{\lambda_{(k_1 \mathbf{k}')} e^{2\pi i k_1 l_1 / N}}{N},$$

where the $\lambda_{(k_1 \mathbf{k}')} = \lambda_{\mathbf{k}}$, $\mathbf{k} \in \mathcal{L}$, are the eigenvalues of V . Now, define the $|\mathcal{L}'| \times |\mathcal{L}'|$ matrices $V(l_1)$ as those matrices obtained from V by keeping the first coordinate fixed: $(V(l_1))_{l'} = V_{(l_1 l')}$. Then the $\lambda_{\mathbf{k}'}(l_1)$ are the eigenvalues of the $V(l_1)$, which are all cyclic and can thus all be diagonalized by the same orthogonal matrix. Choosing \mathcal{O} to be this matrix yields $(\mathcal{O}^t V \mathcal{O})_{(i_1 \mathbf{k}'), (j_1 \mathbf{p}')} = \delta_{\mathbf{k}', \mathbf{p}'} \lambda_{\mathbf{k}'}(i_1 - j_1)$, a *momentum space* representation of the coupling in all but the first coordinate. In this representation the Hamiltonian is a sum of $|\mathcal{L}'|$ mutually uncoupled one-dimensional chains labeled by \mathbf{k}' . Each chain is described by a Hamiltonian of the form as in Eq. (1) with $N \times N$ cyclic coupling matrices $V(\mathbf{k}')$, $(V(\mathbf{k}'))_{l_1} = \lambda_{\mathbf{k}'}(l_1)$. We will write $(V(\varphi'))_{\phi_1} = \lambda_{\varphi'}(\varphi_1)$, $\phi_1 = 2\pi l_1 / N$, $\varphi'_d = 2\pi k'_d / N$, for the infinite system. After this decoupling procedure the entanglement between \mathcal{A} and \mathcal{B} is now given by a sum of the entanglement between the sites $[1, \dots, M]$ and $[M+1, \dots, N]$ of the individual chains:

$$\mathcal{E} = \lim_{N \rightarrow \infty} \sum_{\mathbf{k}'} \frac{E_S(\mathbf{k}')} {N^{D-1}} = \int_{[0, 2\pi]^{\times D-1}} \frac{E_S(\varphi')}{(2\pi)^{D-1}} d\varphi'.$$

This will be the starting point for the following discussion.

Fermions. – We start with investigating case (ii) above: The asymptotic behavior in M after taking the limit $N \rightarrow \infty$ [20], frequently referred to as the *double scaling limit* [17]. For each chain φ' we now need to compute the entanglement between the first M sites and the rest of the chain (in real space,

not momentum space). The asymptotic behavior in M of this entanglement can be obtained from the so-called *symbol* $g_{\varphi}(\varphi_1) = \text{sgn}(\lambda_{\varphi}(\varphi_1))$ of the chain [17, 18]: Each $E_S(\varphi')$ is determined from the continuity properties of $g_{\varphi'}$ as a function of φ_1 . For fixed φ' it corresponds to a one-dimensional isotropic fermionic model, for which the asymptotic form of the entanglement has been obtained in Refs. [17],

$$E_S(\varphi') = \frac{s(\varphi')}{6} \log_2 M + c(\varphi') + o(\log M), \quad (2)$$

where the function $c(\varphi')$ does not depend on M and the integer $s(\varphi')$ is the number of discontinuities of $g_{\varphi'}$ as function of φ_1 in the interval $[0, 2\pi)$. All chains with $s(\varphi') > 0$ are critical as finding discontinuities in the symbol is equivalent to having a vanishing energy gap above the ground state. This means that, depending on the Fermi-surface (the set of solutions to $\lambda_{\varphi} = 0$, see Fig. 1), one finds a continuum of chains φ' that are critical. This situation is in contrast to the situation encountered when considering bosonic systems as we will see below. From (2), we find the asymptotic behavior in M as

$$\mathcal{E} = \frac{\log_2 M}{6} \sum_{\sigma=1}^{\infty} \frac{\sigma v(\Phi_{\sigma})}{(2\pi)^{D-1}} + \int \frac{d\varphi' c(\varphi')}{(2\pi)^{D-1}} + o(\log M), \quad (3)$$

where we defined $v(\Phi_{\sigma}) = \int_{\Phi_{\sigma}} d\varphi'$ as the volume of the set $\Phi_{\sigma} = \{\varphi' : s(\varphi') = \sigma\}$, so the set associated with exactly σ discontinuities. Hence, we do encounter a *logarithmic divergence* in M of the entanglement entropy and the pre-factor depends on the topology of the Fermi-surface: $g_{\varphi'}$ exhibits discontinuities at points where $\lambda_{\varphi} = 0$, i.e., on the Fermi-surface. If the Fermi surface is of measure zero (i.e., the set of solutions to $\lambda_{\varphi} = 0$ is countable, as for example in the critical bosonic case, see Fig. 1), we have $v(\Phi_{\sigma}) = 0$ and the system obeys the area law, $\mathcal{E} = \text{const}$. Consider as an example the case of a nearest neighbor Hamiltonian with coupling $V_{i,j} = \delta_{i,j} + a\delta_{\text{dist}(i,j),1}$, in which case the symbol corresponds for fixed φ' to that of the isotropic XY model with transverse magnetic field $h(\varphi') = 1 + 2a \sum_d \cos(\varphi'_d)$. For this model, the non-leading order term was obtained employing Fisher-Hartwig type methods [17]. It reads $c(\varphi') = \log_2(1 - h^2(\varphi')/4)/6 + c_0$ and vanishes if the chain φ' is non-critical. The constant c_0 is independent of the system parameters. The number of discontinuities is $s(\varphi') = 2$ for

$$\varphi' \in \Phi_2 = \left\{ \varphi' \in [0, 2\pi)^{D-1} : \left| \frac{1}{2a} + \sum_d \cos(\varphi'_d) \right| < 1 \right\}$$

and zero otherwise, i.e., the sum over σ in (3) consists only of the $\sigma = 2$ term as all others are zero. Thus

$$\mathcal{E} = \frac{v(\Phi_2)}{3(2\pi)^{D-1}} \log M + \int_{\Phi_2} \frac{c(\varphi) d\varphi'}{(2\pi)^{D-1}} + o(\log M),$$

where for $D = 2$ and the critical case $|a| > 1/4$, we find $v(\Phi_2) = 2 \arccos(1/(2|a|) - 1)$, i.e., the prefactor depends on the coupling parameter a . For non-critical models in the isotropic setting at hand the set Φ_2 is empty and there is no entanglement. There is no universal non-leading order term

as proposed in Ref. [8] related to the conformal charge, due to the specific geometric setting of a half-space.

At this point, it is interesting to discuss the behavior of the entanglement entropy under *Lifshitz phase transitions*. They are topological quantum phase transitions of fermionic systems due to a change of the topology of the Fermi surface, occurring for example in d -wave superconductors [1], see also Ref. [13]. The previous considerations immediately allow us to argue that a Lifshitz transition accompanied by a change of topology of the Fermi surface is reflected by a non-analyticity in the prefactor $v(\Phi_{\sigma})$ of the entanglement scaling law: Any change of the topology will lead to a non-differentiable alteration of the prefactor of the leading order term.

The second setting is the one of $M = N/2$ (case (i) above), where—in contrast to the double scaling limit— M depends on N , leaving one limit to consider. From the discussion above, we would expect $\mathcal{E} = \infty$. Indeed, making use of a quadratic lower bound to the entanglement entropy [7, 16], it can be shown that fermions violate the area law in this setting: For fermionic models with nearest-neighbor interactions with half-filling in $D = 2$, so $V_{i,j} = a\delta_{\text{dist}(i,j),1}$, we find after some straightforward algebra [21] $\lim_{N \rightarrow \infty} \sum_{k=1}^N E_S(k)/N \geq \lim_{N \rightarrow \infty} \sum_{l=1}^{N/2-1} 4/(\pi^2 l) = \infty$.

Bosons. — We concentrate on the geometrical setting $M = N/2$ (case (i) above) and the most significant model: The D -dimensional free *Klein Gordon field*,

$$\hat{H} = \frac{1}{2} \int_{[0,L]^{\times D}} d\mathbf{r} \left[\pi(\mathbf{r})^2 + \mu^2 \phi(\mathbf{r})^2 + v^2 (\nabla \phi(\mathbf{r}))^2 \right], \quad (4)$$

which may be obtained from a Hamiltonian as in Eq. (1) with a nearest neighbor coupling $V_{i,j} = (\mu^2 + 2D\Omega^2)\delta_{i,j} - \Omega^2\delta_{\text{dist}(i,j),1}$. Denoting the lattice spacing by $\alpha = L/N$ and taking the limit $N \rightarrow \infty$ while keeping $v^2 = \Omega^2\alpha^2$ constant, one obtains (4). Rescaling w.l.o.g. $V \mapsto V/(\mu^2 + 2D\Omega^2)$, we find $V_{i,j} = \delta_{i,j} - c_N\delta_{\text{dist}(i,j),1}$ and $c_N = (\mu^2 L^2/(v^2 N^2) + 2D)^{-1} \xrightarrow{N \rightarrow \infty} 1/2D$. Now, demanding the system to be critical uniquely determines $c_N \rightarrow 1/(2D)$ as the energy gap between the ground and first excited state is given by the square root of the smallest eigenvalue of the coupling matrix V .

For each individual chain \mathbf{k}' , the $V(\mathbf{k}')$ are transformed nearest-neighbor coupling matrices:

$$(V(\mathbf{k}'))_{i,j} = \left[1 - 2c_N \sum_d \cos(2\pi k'_d/N) \right] \delta_{i,j} - c_N \delta_{\text{dist}(i,j),1}.$$

In the infinite system limit, the energy gap $\Delta E(\varphi')$ between the ground and first excited state of each chain is given by $\Delta E(\varphi')^2 D = D - \sum_d \cos(\varphi'_d) - 1$. Hence, in contrast to the critical fermionic case, the set of solutions to $\lambda_{\varphi} = 0$ is of measure zero as only a single chain becomes critical, when we identify 0 with 2π in the spectrum, see Fig. 1. We now make use of a powerful result of Ref. [4]: The exact form of the logarithmic negativity E_n (an upper bound to the entropy of entanglement and an entanglement monotone [22, 23]) with respect to the split $[1, \dots, N/2] || [N/2 + 1, \dots, N]$ for a harmonic chain with nearest neighbor coupling. It is not only an asymptotic statement in N , but a closed-form expression and

we find that $\lim_{N \rightarrow \infty} \sum_{\mathbf{k}'} E_n(\mathbf{k}')/N^{D-1}$ converges to

$$\frac{1}{2(2\pi)^{D-1}} \int_{[0,2\pi]^{D-1}} d\varphi' \log_2 \left(\frac{D - \sum_{d=1}^{D-1} \cos(\varphi'_d) + 1}{D - \sum_{d=1}^{D-1} \cos(\varphi'_d) - 1} \right) \geq \mathcal{E},$$

independent of the mass μ . For $D = 2$ it evaluates to $\log_2(3 + 2\sqrt{2})/2$ and similarly for $D > 2$. Hence, the entanglement entropy for this critical model is bounded by an expression linear in the *boundary area*, we do not encounter an infrared divergence here, and the prefactor can be exactly determined for the logarithmic negativity.

Summary. – In this work, we have clarified the issue of scaling of the entanglement entropy in bosonic and fermionic lattice systems. Our analytical argument indeed confirms and resolves previous numerical findings and conjectures on the scaling of entanglement in ground states of many-body systems. The difference between the behavior of bosons and fermions may be taken as unexpected. A new length scale emerges that can be referred to as “entanglement thickness”: This length scale is associated with the possibility of approximately disentangling the two regions with local operations. As a pure Gaussian state is equivalent to a product of two-

mode squeezed states up to local unitary rotations, one finds that this scale is in fact associated with the lattice spacing, and not the correlation length. The violation of the area-law for fermions is in fact intertwined with the specific role of the Fermi surface. We found that quantum phase transitions involving an alteration of the topology of the Fermi surface result in a non-analytical behavior of the prefactor.

For typical critical models we found that those individual boundary crossing chains obtained from our decoupling procedure that are critical form a continuum for fermions and are finite in number for bosons. Integrating over all chains then “lifts” singularities in $D > 1$ for bosons. For critical bosonic models exhibiting only a finite number of ground states, one might expect that an area law holds in dimensions $D > 1$ even for models that go beyond quadratic Hamiltonians considered here and are thus truly interacting. Confirming or refuting this conjecture is an interesting challenge.

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 - [20] Considering the entanglement of a single site with the rest, we find $E_S = (\varrho_F - 1) \log_2(1 - \varrho_F) - \varrho_F \log_2(\varrho_F)$, which is equal to zero for non-critical systems ($\lambda_k < 0$ or $\lambda_k > 0$), maximal for half filling, and independent of N , thereby allowing for a meaningful study of the scaling of entanglement in M after letting $N \rightarrow \infty$. Here, the filling factor is given by $\varrho_F = \frac{1}{2} - \sum_{\mathbf{k}} \text{sgn}(\lambda_{\mathbf{k}})/(2N^D)$. For critical bosons in $D = 1$ this entanglement diverges in N , i.e., the scaling in the size of \mathcal{A} after letting $N \rightarrow \infty$ is not well defined – a manifestation of the *infrared divergence* in $D = 1$ [2].
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